Supplementary Material for: Safeguarding drinking water in North-Western Europe by modelling the fate of amines from CO_2 capture

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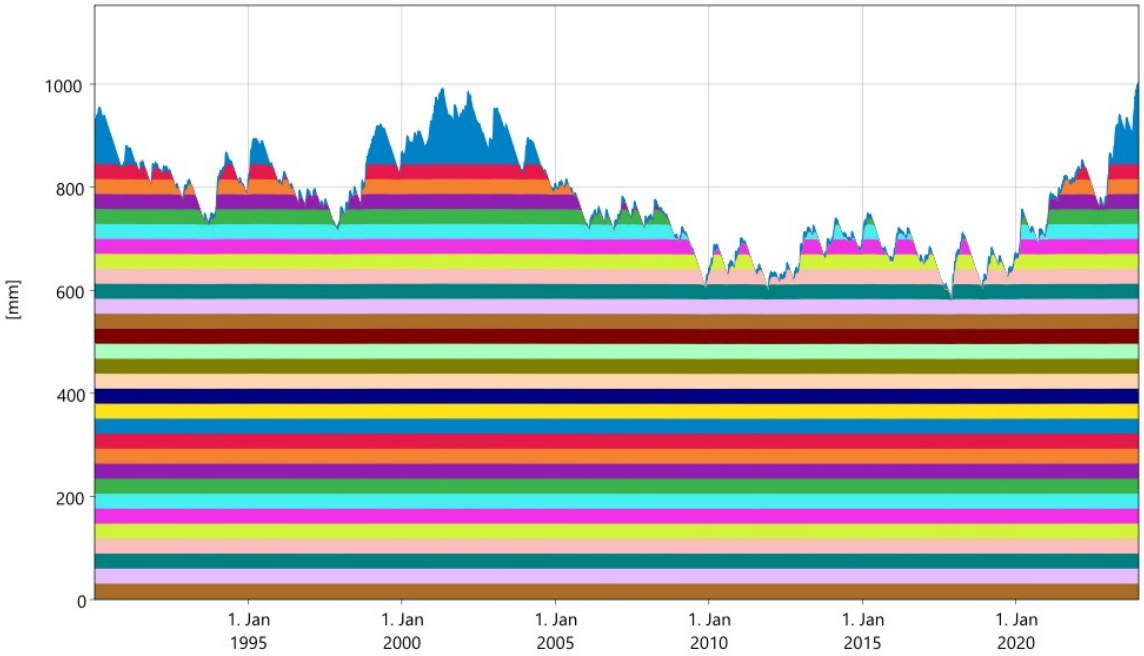

FigureS1: Modeled groundwater level in Sint Jansteen aquifer across the thirty layers.

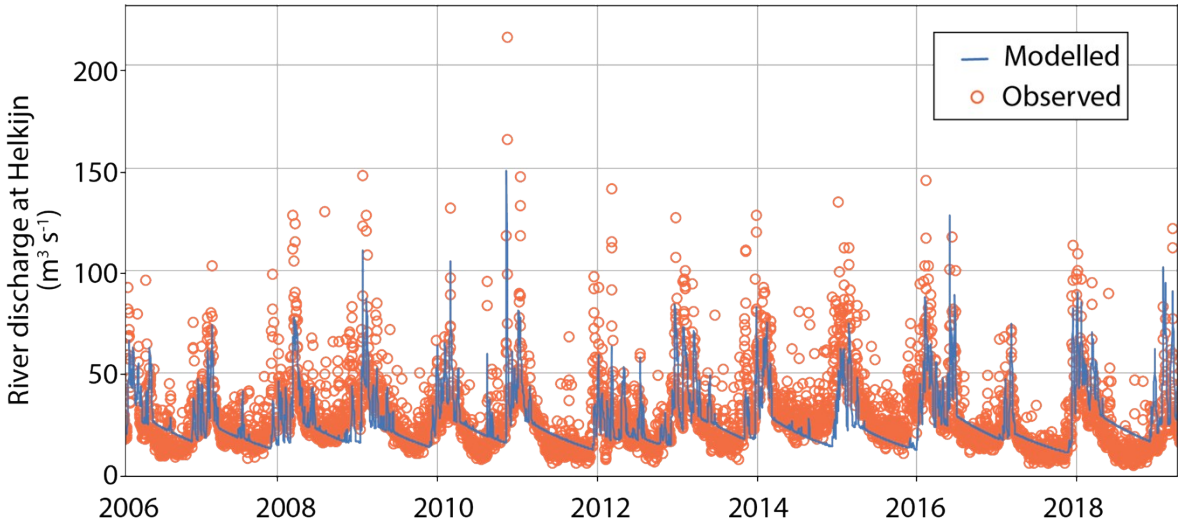

Figure S2: Comparison of modelled and observed river discharge in the Schelde River at Helkijn station.

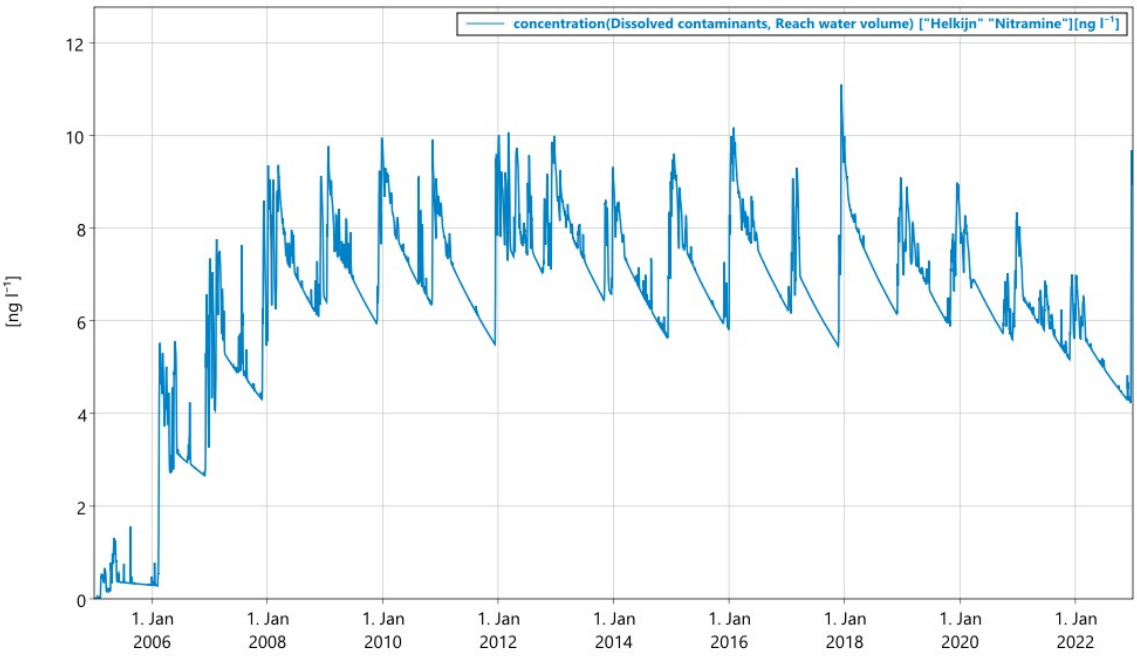

Figure S3: Modelled NA+NSA concentrations in the Schelde river (deposition rate: 8 ng m^{-2} day^{-1}, NA+NSA half-life: 2 yr)

Table S1: Surface and groundwater model parameters

		Value	
NA and NSA physical properties	**Units**	**NSA**	**NA**
Molar mass [1]	g mol^{-1}	74.1	90.7
Molecular volume [1]	cm^3 mol^{-1}	56.5	90.7
Henry's constant at 25°C [1]	Pa m^3 mol^{-1}	0.104	0.081
Log10 Octanol-water partitioning coefficient [1]	-	-0.7	-0.9
Surface water model parameters	**Units**	**Value**	
Degree-day evapotranspiration [auto-calibrated]	mm $°C^{-1}$ day^{-1}	0.18	
Baseflow index [auto-calibrated]	-	0.75	
Shallow soil water time constant [auto-calibrated]	days	8	
Shallow soil field capacity [auto-calibrated]	mm	290	
Deep soil temperature [fixed]	°C	8	
Deep soil time constant [auto-calibrated]	days	400	
Shallow soil solid organic carbon [fixed]	kg m^{-2}	30	
Deep soil solid organic carbon [fixed]	kg m^{-2}	3	
Shallow soil dissolved organic carbon [fixed]	mg L^{-1}	10	
Deep soil dissolved organic carbon [fixed]	mg L^{-1}	10	
Groundwater model parameters	**Units**	**Value**	
Baseflow index [fixed]	-	0.69	
Soil water time constant [fixed]	days	2	
Soil field capacity [fixed]	mm	120	
Groundwater temperature [fixed]	°C	8	
Groundwater travel time [resulting from calibration]	years	5 or 10	
Groundwater layer field capacity [calibrated]	mm	29.2 or 58.3	
Degree-day evapotranspiration [fixed]	mm $°C^{-1}$ day^{-1}	0.14	
Soil solid organic carbon [fixed]	kg m^{-2}	30	
Groundwater solid organic carbon [fixed]	kg m^{-2}	3	
Soil dissolved organic carbon [fixed]	mg L^{-1}	6	
Groundwater dissolved organic carbon [fixed]	mg L^{-1}	3	

Reference: [1] Brecke Gundersen et al. (2024)

Table S2: Calibration statistics for river water flow predictions in Schelde River.

Statistics	Daily
NSE	0.50
KGE	0.65
R^2	0.51
Spearman Rank Correlation	0.55
Bias	0.86 $m^3 s^{-1}$
RMSE	13.50 $m^3 s^{-1}$
RSR	0.71
PBIAS	3.0%

NSE: Nash-Sutcliffe efficiency; KGE: Kling-Gupta efficiency; RMSE: root mean squared error; RSR: RMSE-observations standard deviation ratio (Moriasi et al. 2007); PBIAS: Percent bias (Moriasi et al. 2007).

References:

Gundersen, C. B., Norling, M. D., & Gragne, A. S. (2024). Modelling future levels of nitrosamines and nitramines in a groundwater compartment close to a CO2 capture facility. In 27. Norsk institutt for vannforskning. https://niva.brage.unit.no/niva-xmlui/handle/11250/3160694

Moriasi, D., Arnold, J., Van Liew, M., Bingner, R., Harmel, R. D., & Veith, T. (2007). Model Evaluation Guidelines for Systematic Quantification of Accuracy in Watershed Simulations. Transactions of the ASABE, 50. https://doi.org/10.13031/2013.23153